CHARACTERIZATION OF THE FLOW FIELD AND WIND SPEED PROFILES IN MICROBALANCE WIND TUNNELS FOR MEASUREMENT OF AGENT FATE

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ABSTRACT

An important goal is to model chemical warfare agent fate on environmental and interior surfaces and therefore, rigorously measured evaporation and desorption rates are required to develop equations for these transport processes. A difficult problem in environmental fate research is the assignment of a wind speed to an evaporation or desorption process for a droplet. The average wind speed is recorded, but the wind speed controlling the transport of liquid to vapor at the droplet interface at ground level is a much lower value. The wind speed profiles in several microbalance wind tunnel geometries were measured in order to assign an appropriate wind speed to the chemical agent evaporation rates measured. Both hot wire anemometry and computational fluid dynamics were employed to characterize the flow field in the microbalances. Separate inlet geometries were compared since low and high humidity air can have different inlet flow paths. The characterization of a dual microbalance with differential weight loss and differential temperature measurement capability was added to the preliminary characterization of single beam microbalances studied previously.

INTRODUCTION

Understanding the evaporative properties of different chemical agents as a function of the ambient air's humidity, temperature and wind speed is important to the development of accurate hazardous prediction computer models, such as VLSTRACK and HPAC. In order to obtain this information, several different analytical methods, such as small-scale laboratory experiments, larger scale wind tunnels studies and open-air field tests, are being pursued simultaneously. Variables that control the evaporation or desorption of liquid contaminants include temperature, relative humidity, drop size, and wind speed. The goal of this investigation is to characterize the flow field and wind speed within laboratory thermal gravimetric analyzers (TGA); three different sample geometries and flow paths were studied. The conventional use of the TGA is the measurement of reactive or desorption processes. In order to measure the environmental fate of toxic chemical from material surfaces, we have converted the TGA instruments into microbalance wind tunnels (Ref 1). Environmental fate wind tunnels require the characterization of the wind speed near the surface where the toxic droplet is evaporating or desorbing. Because the wind speed near the chemical droplet being studied is an important factor in determining evaporation rates, the velocity profiles above the sample pans were measured experimentally and simulated computationally. Due to the extremely low flow rates and the small cross-sectional area at the sample location,

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experimental measurements were extremely difficult. This difficulty led to a balanced strategy of employing both experimentation and Computational Fluid Dynamic (CFD) simulations of the flow field over the sample pans, with the experimental measurements serving as a means of validating the simulations (Ref 2). Results from these measurements and simulations are presented in this paper.

EQUIPMENT AND PROCEDURES: MICROBALANCE WIND TUNNELS

For this study, conventional laboratory TGA instruments were converted into microbalance wind tunnels. In general, a TGA is a device that uses a very sensitive electronic micro-gram balance to record the change in mass of the chemical test droplet on various substrate materials as a function of time for independent variables of wind speed, drop size, temperature and humidity. Although three different microbalance instruments were used in this study, and each differs in design, their overall operation is approximately similar. Typically, the surface material specimen is placed in the sample pan, for example: concrete, aggregate, asphalt, grass, soil, etc.; the sample pan is suspended from the end of the microbalance beam. The microbalance beam is a rod that extends from the microbalance mechanism into the middle of a furnace tube. The conditioned test gas flows through this tube over the chemical droplet, which has been placed on the material surface. The evaporation or desorption of the chemical droplet is measured vs. elapsed time, while maintaining the test gas at constant humidity and temperature. The three different model TGA instruments employed as microbalance wind tunnels were manufactured by TA Instruments, Inc (New Castle, DE) and the characterization of each is described below.

MODEL TA 2950 GEOMETRY

The model TA 2950 microbalance is oriented vertically, with the sample pan hung near the bottom of a larger diameter glass tube; a smaller tube provides gas flow across the sample pan in the Evolved Gas Analysis mode, see Figure 1. Ninety percent of the primary flow passes through this small side tube over the sample pan, and 10% flows down the larger tube to prevent hazardous vapor from entering the microbalance mechanism. For the model 2950, primary flow rates of 0.09, 0.6 and 1.2 L/min were studied. In typical operations the tube shown in Figure 1 is enclosed inside of a furnace heating element, which maintains a constant gas and sample temperature as it flows over the sample pan. The primary flow tube has a diameter of approximately 4mm. Due to the difficulty in supplying the secondary 10% flow in the experimental setup, only the primary flow was used in making the hotwire measurements. However, the secondary flow was modeled in the CFD simulations.

MODEL TA 951 GEOMETRY

The model 951 TGA uses a horizontally oriented microbalance. The sample pan hangs below the microbalance beam, which is positioned inside of a 23mm diameter horizontal flow tube. For the micro wind tunnel application a study was conducted with a longer than normal quartz flow tube in order to improve the flow quality near the sample pan. Figure 2 shows the experimental setup for the model 951 TGA boundary-layer profile measurements above the sample pan. Five different flow rates were studied: 0.6, 1.2, 2.4, 3.6 and 4.8 L/min.

A modified version of the Model 951 was also designed and studied computationally. This modified design incorporated a vacuum plenum around the flow tube, thus allowing the test gas to flow from both directions, keeping the microbalance mechanism clean of hazardous chemical vapors. The modified Model 951 flow tube is illustrated in Figure 3.

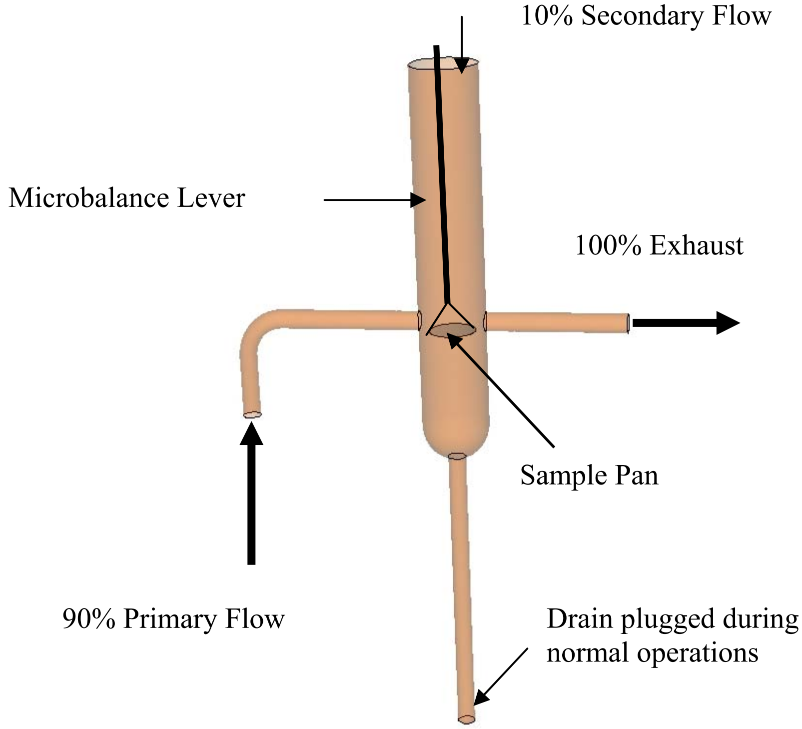

Figure 1 TGA Model TA 2950 CFD geometry

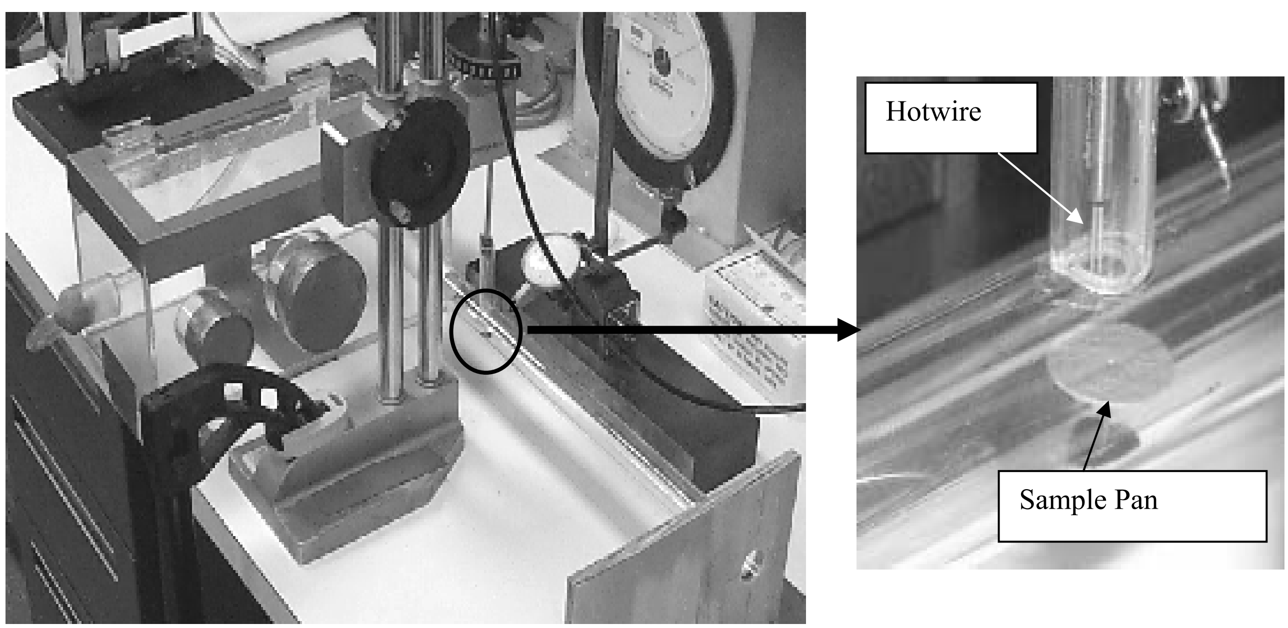

Figure 2 TGA Model 951 Experimental Setup; the insert shows sample pan and hotwire probe.

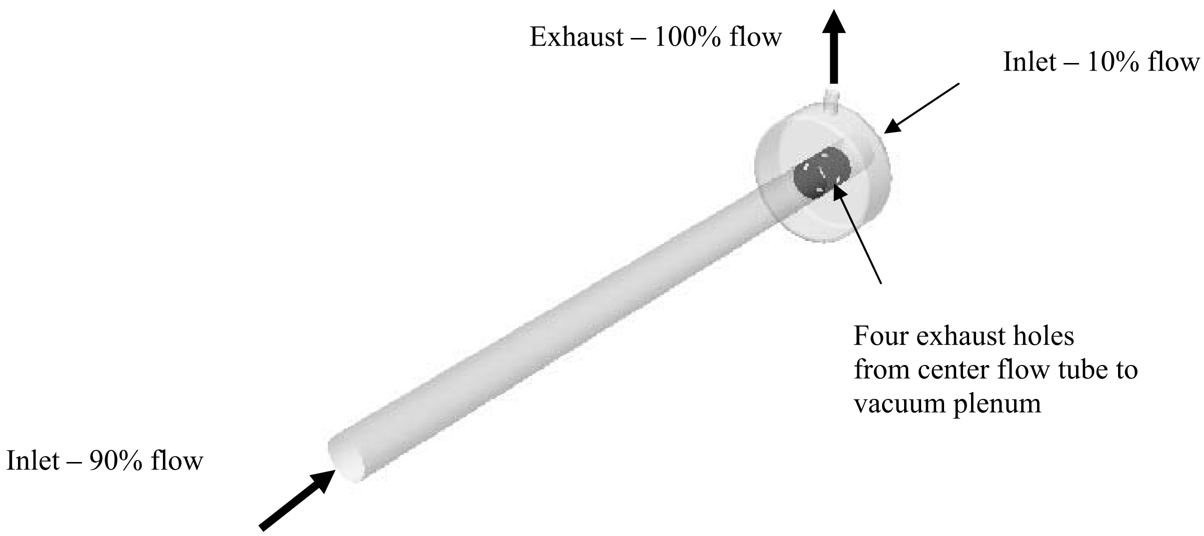

Figure 3 Modified TGA model 951 design

MODEL TA Q600 GEOMETRY

The Model TA Q600 device is similar to the Model 951, except that it uses twin, horizontal microbalances, with differential thermal measurements between each sample. The two microbalances permit two substrates to be evaluated simultaneously within the same environment with one substrate serving as a control and the other use to evaluate chemical droplet. The flow rates range for this instrument is 0.1 to 1 Lpm; however, these flow rates were below the calibration limits of the hotwire used to measure the boundary-layer profiles above the sampling pan. Therefore, higher flow rates of 2.0, 3.0 and 4.0 Lpm were used for the experimental study. These experimental results were then used to compare to the CFD simulation results, which covered the full range of flow rates and wind speeds. Figure 4 shows the internal components of the Model Q600, including the 23mm diameter flow tube.

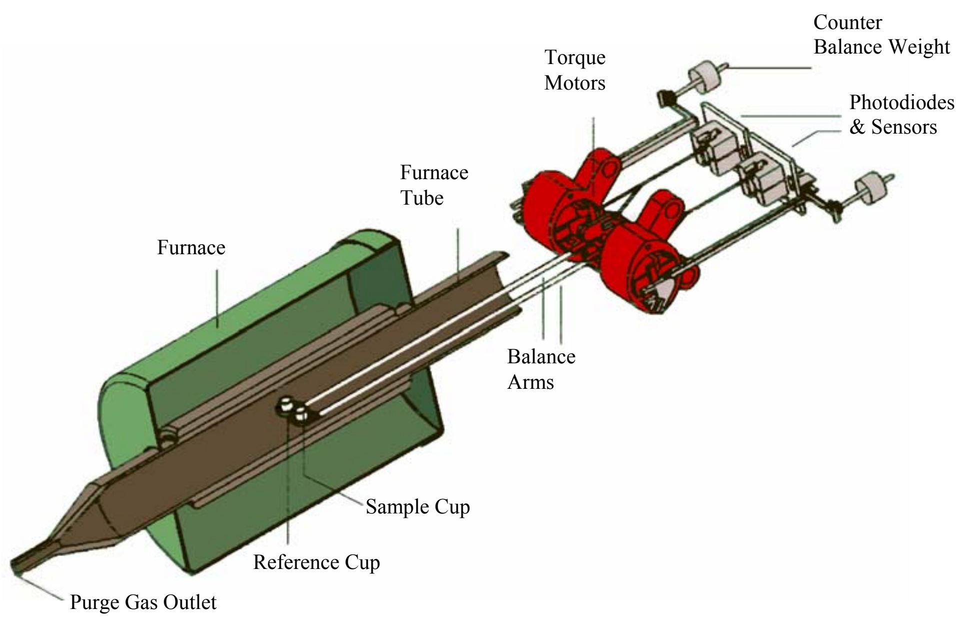

Figure 4 TGA Model Q600 internal schematic components.

FLOW FIELD AND WIND SPEED MEASUREMENTS

Numerous experimental measurements were performed on each of the microbalance wind tunnel models to quantify and characterize the boundary-layer profiles above the sample pan. Velocity and turbulence intensity were measured using a constant temperature hot-film anemometer (IFA-300 system; TSI, Minneapolis, MN). Special care was taken to extend the hotwire probe calibration down to 0.05 m/s in order to cover the expected low speeds near the sample pan surface. Velocity profiles and turbulence intensity measurements were performed from within approximately 0.254mm of the sample pan to near the top of the tube. The hot wire anemometer probes were mounted on a high precision, low compliance micro-positioning instrument. For most tests, a small vacuum pump (connected to a plenum to dampen flow variations) and a Dry Cell flow meter were used to set the appropriate test flow rate.

COMPUTATIONAL PROCEDURES

The CFX CFD program version 5.6 (Ansys Ltd., Pittsburgh, PA) was used to simulate the flow in the various microbalance wind tunnel geometries. CFX creates an unstructured mesh and uses a coupled solver to simulate the flow field on the mesh. A variety of graphic output options were employed for data presentation.

RESULTS: EXPERIMENTAL AND COMPUTATIONAL

TGA MODEL 2950

Experimental boundary-layer measurements on the quartz flow tube of the Model 2950 were extremely difficult to make due to the low flow rates and small size of the flow tube. Velocity profile measurements were made without a sample pan installed, and boundary-layer measurements were made with a sample pan installed for flow rates of 0.09, 0.6 and 1.2 L/min. Computational modeling was performed at the same flow rates. A comparison of the results is shown in Figure 5.

Agreement between the experimental and computational results is good at 0.09 and 0.6 Lpm. For the 1.2 Lpm flow rate, the experimental results indicate a fluctuation in the velocity profile, which is not present in the computation results. Intuition would suggest that the profile should be similar to the CFD prediction; however, the reason for the fluctuation in the experimental results is not understood at this time. Overall the agreement between the experimental and CFD results was quite good. An important measurement is at the lowest height, 0.25 mm (0.01 inch), since this value is closest to the interface between the chemical droplet and material surface. Both the experimental and computed velocities converge at about 0.3 m/s at 0.25 mm for the 0.6 Lpm flow case. Note that this 0.3 m/s (0.7 mph) is much less than the mean wind speed of 0.9 m/s (2.0 mph) or a maximum near-centerline measurement of about 1.3 m/s (2.9 mph). As noted previously only the primary flow was used for the experimental measurements, but both the primary and secondary flows were modeled in the CFD simulations. Three-dimensional representations of the merger of the horizontal (primary) and vertical (secondary) flows were obtained from the CFD simulations and showed that most of the vertical (secondary) flow remained close to the tubing wall of the exit port, as reported previously (Ref 2).

TGA MODEL 951

Boundary-layer measurements and computational simulations were performed using a simulated wind tunnel flow tube and sample tray (see Figure 2) for flow rates of 0.6, 1.2, 2.4, 3.6 and 4.8.Lpm. A comparison between the computational and experimental results is shown in Figure 6.

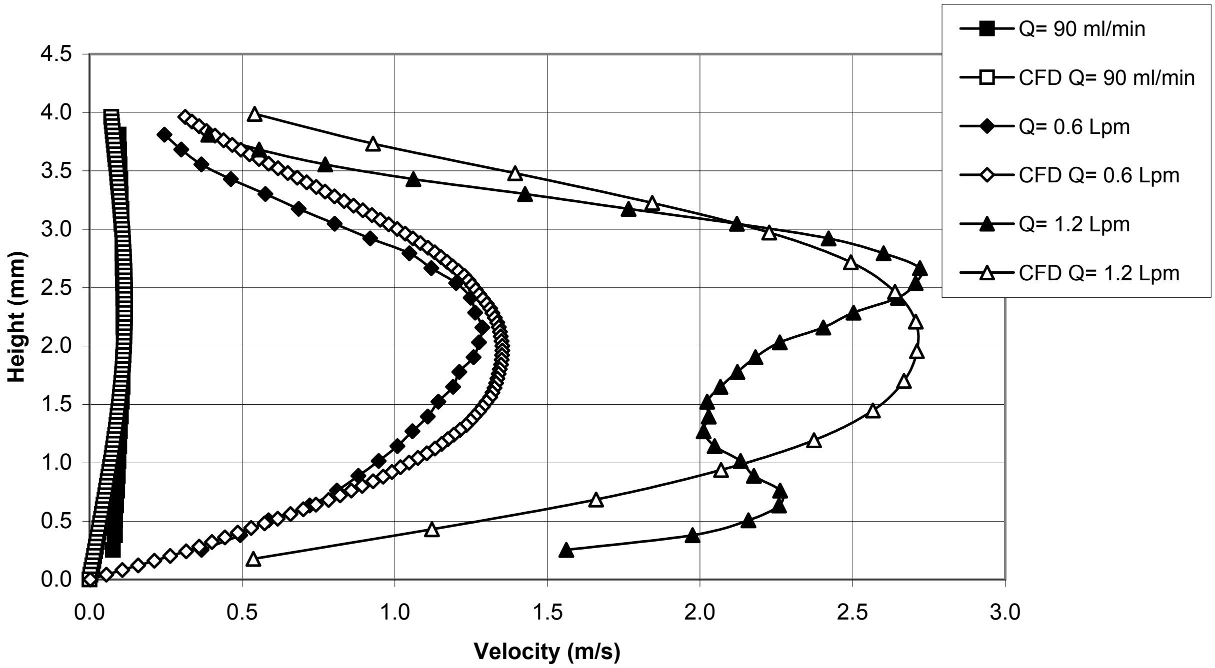

Figure 5. Comparison of experimental and computational results for TGA Model TA 2950 (1 m/s = 2.2 mph)

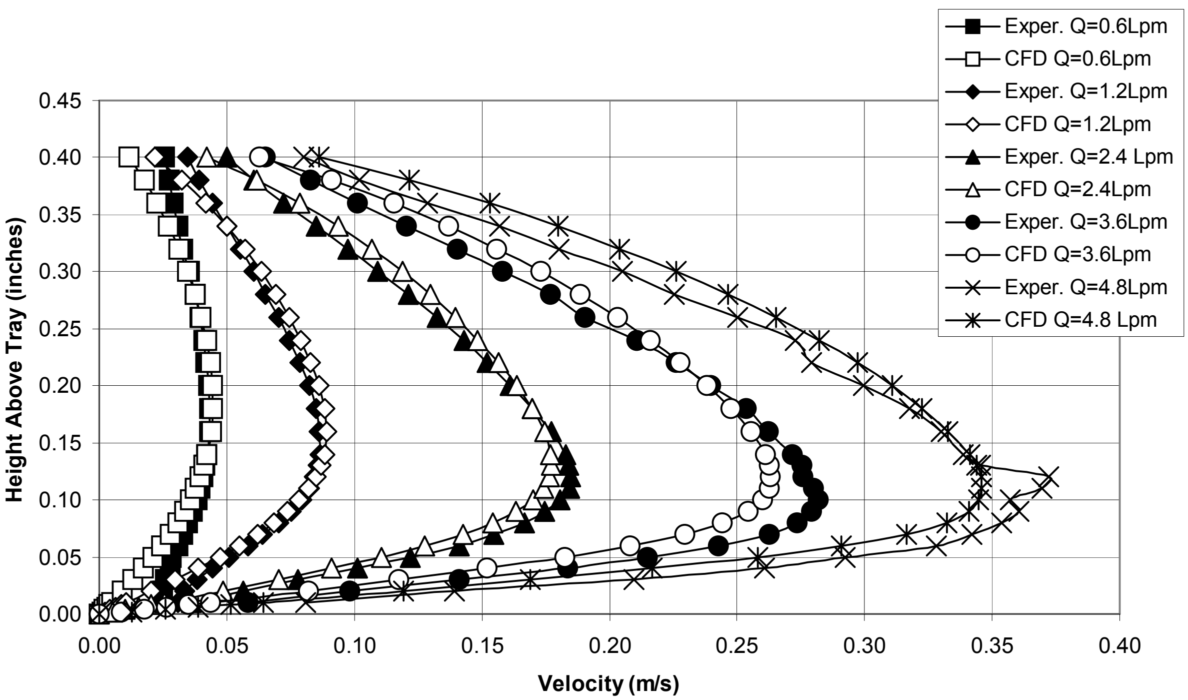

Figure 6 Comparison of experimental and CFD results for TGA Model 951

The comparison of the experimental to CFD boundary-layer profiles is very good. Note that the 0.25 mm height wind speeds are less than 0.05 m/s (0.11 mph) while use of the mean wind speed for a flow rate of 4.8 Lpm results in an wind speed of 0.21 m/s (0.47 mph), and the max speed is approximately 0.35 m/s therefore, the actual wind speed near the interface is several times lower than a simplistic value from

the cross-section and flow rate calculation. Because of the good agreement between experimental and simulation, the CFD could be used to simulate the boundary-layer growth over the centerline of the sample pan in the direction of the flow, especially due to the difficulty in trying to experimentally measure the profiles other than those at the center of the pan. The CFD boundary-layer growth approximation for the 3.6 Lpm flow rate is shown in Figure 7. As expected, the boundary-layer is small at the upstream edge of the pan and grows towards the downwind side. At the center (50% of sample pan diameter) the boundary-layer is approximately 2.8mm, or 74% of the full boundary layer thickness. As an example of an application of the result, one would limit droplet placement to avoid the front 20-30% of the sample pan, where the steep, low velocity profile exists.

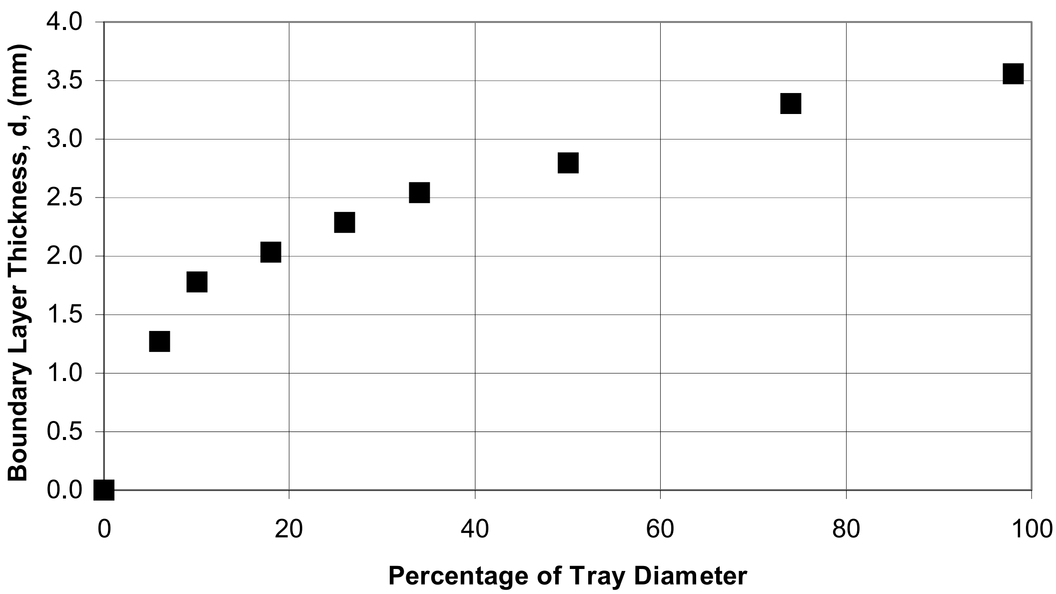

Figure 7 CFD Simulation Of Boundary-Layer Growth Across The Sample Pan Of The Model 951 At 3.6 Lpm

TGA MODEL Q600

The final TGA model study for use as a micro wind tunnel was the Model Q600. To date experimental results have been obtained for the 2.0, 3.0 and 4.0 Lpm flow rates, and computational simulations have been conducted for the 0.1, 1.0 2.0, 3.0 and 4.0 Lpm cases. As pointed out above, the higher flow rates in the experimental study were necessary because of the corresponding low velocities and the lower measurement threshold of the hotwire anemometer. Figure 8 shows a comparison of the experimental and CFD results. The shape of the experimental and CFD profiles are in fair agreement, but the magnitudes of the results are not. The reason for this discrepancy is not known at this time. Once good agreement is achieved between the experimental and CFD results at the higher flow rates, CFD simulations will be used to simulate the more realistic lower flow rates.

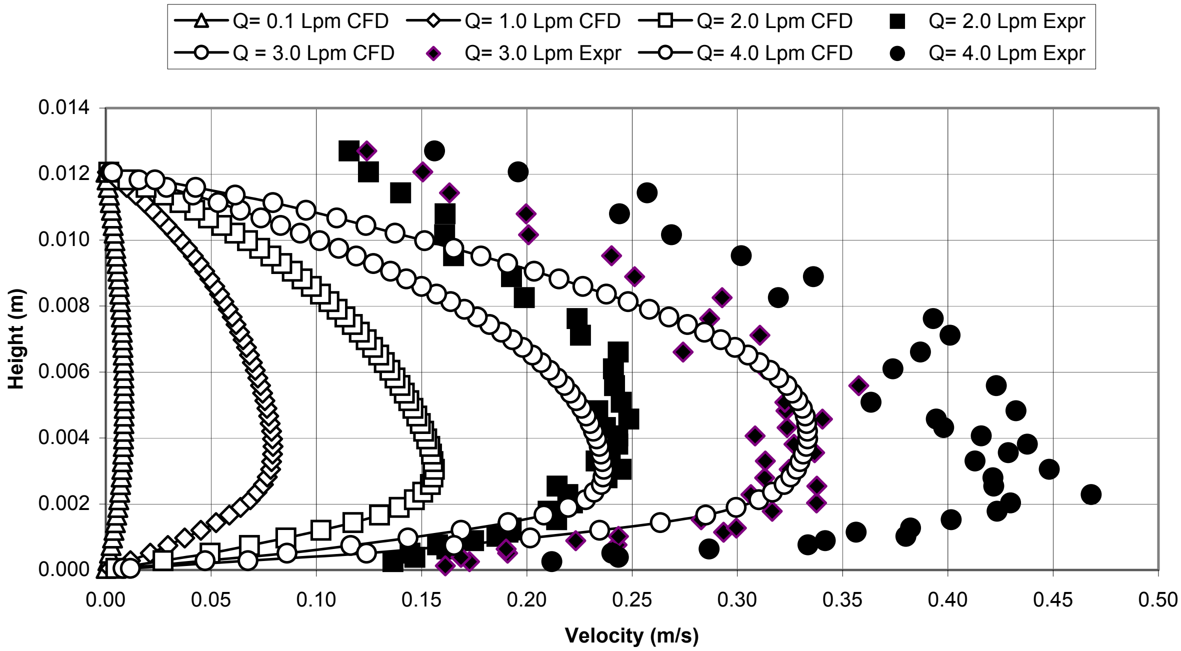

Figure 8. TGA Model Q600 Comparison Of Experimental And CFD Of The Boundary-Layer Above The Sample Pan As A Function Of Flow Rate: wind speed near the chemical-material interface at a 0.25 mm height is less than 0.05 m/s (0.11 mph).

CONCLUSIONS

Thermal microbalance instruments were configured as microbalance wind tunnels for the measurement of evaporation and desorption of toxic chemical droplets form materials surfaces under environmental conditions; these measurements are currently being performed successfully. The environmental wind speed is one of the variables to be evaluated. The mean wind speed obtained from the flow rate and cross-sectional area has been employed previously. Improved flow field characterizations are being obtained using a precision micro-positioning device, subminiature hotwire anemometer probes, and computational fluid dynamic simulations to measure and compute the wind speed near the chemical-material surface interface. In general, the height above the surface at and below 0.25 mm (0.01 inch) extended below the viscous sublayer for most surface roughness lengths, and the wind speed ranges measured were at or above the friction velocities for concrete through cropped grass (Ref 3). Therefore, the microbalance wind tunnels can be configured to cover most of the experimental conditions in an environmental test matrix.

In preliminary studies of the Model TA 2950 geometry using miniature hotwire probes, the experimental and computation profile results were in good agreement. Experimental and computational agreement was also good for the TA 951. To date, there is a discrepancy in the agreement between the velocity magnitude of the experimental (performed with subminiature hotwire probes) and computational profile results for the Q600. Work continues to identify the cause of this discrepancy. Once identified and corrected, the expanded use of CFD simulations to obtain flow field information that was too difficult to obtain experimentally will be permitted.

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